

Resonant Inelastic X-ray Scattering Study of CuO

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Introduction: The electronic structure of superconducting cuprates and transition metal oxides is a topic of high interest in solid state physics. Recent measurements of the energy loss spectra of Nd_2CuO_4 [1], La_2CuO_4 [2], $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ [3] and CuO [4] using resonant inelastic scattering spectroscopy (RIXS) gave rise to some discussion as the results of the latter three experiments are to some extent contradictory to the results of the first one. A feature at an energy loss of about 5 eV, which is attributed to a shake-up process in the intermediate core-hole state of the resonant scattering process, is seen in each of the four experiments. But only the spectra of the latter three show an evident dependence of the feature's intensity on the momentum transfer vector \mathbf{q} while the measurements on Nd_2CuO_4 show no such effect.

Methods and Materials: For a better insight into the scattering process which leads to the shake-up feature we have repeated the experiment on CuO in a different scattering geometry. Earlier measurements on the same substance have been performed in a geometry where the incident photon's polarisation vector \mathbf{e}_1 is parallel to the scattering plane (horizontal geometry). To achieve a better comparability between the results for CuO and for Nd_2CuO_4 we now chose a geometry where \mathbf{e}_1 is perpendicular to the scattering plane (vertical geometry) as in the case of Nd_2CuO_4 . Furthermore we aligned the CuO single crystal in a way that \mathbf{e}_1 is parallel to the CuO_2 planes inherent to the crystal. In the first part of the experiment we then measured the energy loss spectra of CuO between 0 eV and 15 eV of energy loss for a fixed excitation energy of 8986 eV and for three different scattering angles of 90, 120 and 130 degrees. In the second part of the experiment we measured the same energy loss spectra but now for a fixed scattering angle of 90 degrees and for different excitation energies between 8978 eV and 9004 eV.

Results: The results of the first part of the experiment are shown in Fig. 1. One can clearly see that the intensity of the shake-up feature at an energy loss of 5 eV doesn't change its intensity as a function of the scattering angle and therefore as a function of \mathbf{q} . This result is in agreement with the results of the Nd_2CuO_4 experiment but contradicts the findings of earlier measurements on CuO but for the horizontal scattering geometry. To explain the different behaviour in both geometries we studied the polarisation dependence of the shake-up feature using a model based on the polarisation dependence of the resonant elastic scattering amplitude. We found that the change of the feature's intensity as a function of the scattering angle in the horizontal geometry can be explained by the change of the scattered photon's polarisation vector \mathbf{e}_2 with respect to the coordinate system of the CuO crystal. Within this model no such effect is expected to show up in vertical scattering geometry which is in agreement with the experimental findings. Therefore we conclude that the process related to the shake-up feature in the energy loss spectrum of CuO is a local excitation of the electronic system showing no \mathbf{q} -dependence but only a polarisation dependence in horizontal scattering geometry.

Fig. 2 shows the results of the second part of the experiment. Obviously the shake-up satellite is not present for arbitrary excitation energies but shows two resonances which can be related to different intermediate core-hole states.

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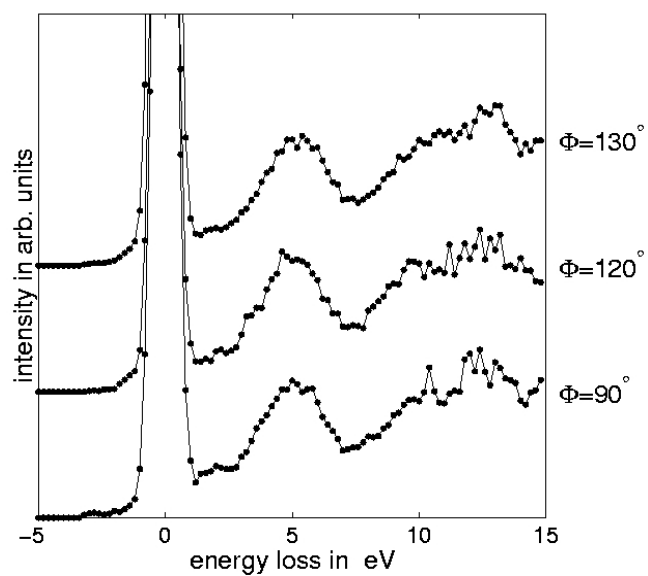


Fig. 1: Energy loss spectrum of CuO with an excitation energy of 8986 eV for three different scattering angles. The shake-up feature at 5 eV of energy loss shows no change in its intensity.

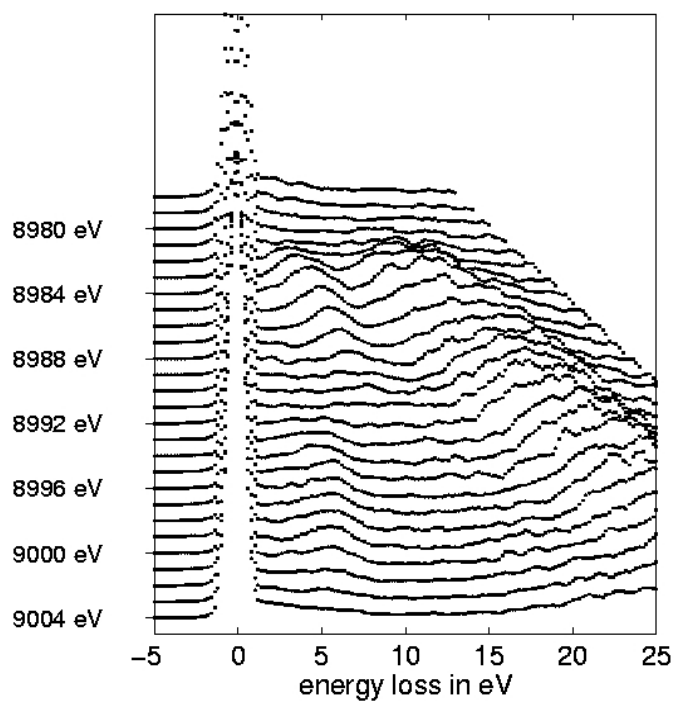


Fig. 2: Energy loss spectrum of CuO for different values of the excitation energy E_0 , given on the left side. The shake-up feature is only present between $8982 \text{ eV} < E_0 < 8990 \text{ eV}$ and again between $8993 \text{ eV} < E_0 < 9002 \text{ eV}$.